10/552,595D part 04/24/2009 Yong Chu

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SESSION RESUMED IN FILE 'REGISTRY' AT 10:32:38 ON 24 APR 2009
FILE 'REGISTRY' ENTERED AT 10:32:38 ON 24 APR 2009
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COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 210.84 211.06

=> d his

     (FILE 'HOME' ENTERED AT 09:51:22 ON 24 APR 2009)

     FILE 'REGISTRY' ENTERED AT 09:51:38 ON 24 APR 2009
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 STRUCTURE UPLOADED
L4 12498 S L1 FULL
    SAVE L4 YC10552595 7A
L5 STRUCTURE UPLOADED
L6 STRUCTURE UPLOADED
L7 STRUCTURE UPLOADED

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 211.32 211.54

FILE 'REGISTRY' ENTERED AT 10:33:00 ON 24 APR 2009
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STRUCTURE FILE UPDATES: 22 APR 2009 HIGHEST RN 1138219-76-7
DICTIONARY FILE UPDATES: 22 APR 2009 HIGHEST RN 1138219-76-7

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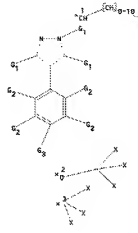
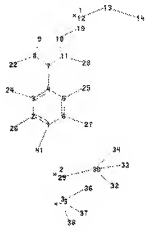
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10552595\L14_04242009.str





chain nodes :
12 13 14 19 20 22 24 25 26 27 29 30 32 33 34 35 36 37 38 41
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
1-41 2-26 3-24 4-7 5-25 6-27 8-22 10-19 11-20 12-13 13-14 29-30 30-32
30-33 30-34 35-36 35-37 35-38
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11
exact/norm bonds :
1-41 2-26 3-24 5-25 6-27 7-8 7-11 8-9 8-22 9-10 10-11 10-19 11-20 29-
30

exact bonds :
4-7 12-13 13-14 30-32 30-33 30-34 35-36 35-37 35-38
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:CH3,H,[*1]

G2:H,CH3

G3:G1,OH,SH,CN,NH2,NO2,X,[*2],[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 19:CLASS 20:CLASS 22:CLASS 24:CLASS
25:CLASS 26:CLASS
27:CLASS 29:CLASS 30:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:CLASS 38:CLASS
41:CLASS

```
L8       STRUCTURE UPLOADED
```

```
=> d
L8 HAS NO ANSWERS
L8               STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l8 sam sss sub=l4
SAMPLE SUBSET SEARCH INITIATED 10:33:38 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -      639 TO ITERATE

100.0% PROCESSED      639 ITERATIONS                              3 ANSWERS
SEARCH TIME: 00.00.01

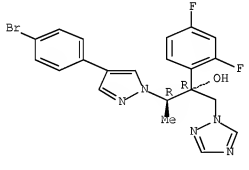
PROJECTIONS (WITHIN SPECIFIED SUBSET):          ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):       11264 TO    14296
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):              3 TO      163

L9            3 SEA SUB=L4 SSS SAM L8

=> d scan

L9   3 ANSWERS   REGISTRY  COPYRIGHT 2009 ACS on STN
IN   1H-1,2,4-Triazole-1-ethanol, .alpha.-[(1R)-1-[4-(4-bromophenyl)-1H-pyrazol-
     1-yl]ethyl]-.alpha.-(2,4-difluorophenyl)-, (.alpha.R)-
MF   C21 H18 Br F2 N5 O

Absolute stereochemistry.
```

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> s l8 full sss sub=l4
FULL SUBSET SEARCH INITIATED 10:34:21 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -     12498 TO ITERATE
```

100.0% PROCESSED 12498 ITERATIONS 59 ANSWERS
SEARCH TIME: 00.00.01

L10 59 SEA SUB=L4 SSS FUL L8

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 44.96 256.50

FILE 'CAPLUS' ENTERED AT 10:34:26 ON 24 APR 2009
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FILE COVERS 1907 - 24 Apr 2009 VOL 150 ISS 18
FILE LAST UPDATED: 23 Apr 2009 (20090423/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l10
L11 41 L10

=> save l11
ENTER NAME OR (END):yc10552595A/A
ANSWER SET L11 HAS BEEN SAVED AS 'YC10552595A/A'

=> d ibib abb hitstr 30-41
'ABB' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing

```
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
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FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

=> d ibib abs hitstr 30-41

L11  ANSWER 30 OF 41  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:         1981:568095  CAPLUS  Full-text
DOCUMENT NUMBER:          95:168095
ORIGINAL REFERENCE NO.:   95:28085a,28088a
TITLE:                    Free-radical reactions of diazonium salts with
                          .alpha.,.beta.-unsaturated carbonyl compounds.  A new
                          synthesis of 1,4-diarylpyrazole derivatives
```

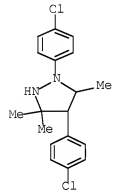
AUTHOR(S): Citterio, Attilio; Ramperti, Massimo; Vismara, Elena
CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy
SOURCE: Journal of Heterocyclic Chemistry (1981), 18(4), 763-6
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:168095

AB Free-radical decompn. of benzene diazonium salts catalyzed by titanous or titanous and ferrous salts in th presence of .beta.-substituted .alpha.,.beta.-unsatd. carbonyl compds., e.g., 4-methyl-3-pentene-2-one, Me 2-butenoate, leads to 1,4-diarylpyrazole derivs. The reaction occurs via an intermediate azo compds., which can be reduced by the metal salt or can be isolated and hydrogenated to pyrazole derivs.

IT 79481-66-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 79481-66-6 CAPLUS

CN Pyrazolidine, 1,4-bis(4-chlorophenyl)-3,3,5-trimethyl- (CA INDEX NAME)

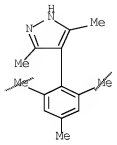


L11 ANSWER 31 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1976:179094 CAPLUS Full-text
DOCUMENT NUMBER: 84:179094
ORIGINAL REFERENCE NO.: 84:29023a,29026a
TITLE: Anisotropy effects of conjugated cyclic systems, I. NMR spectra of mesityl- and (9-anthryl)-substituted aromatic compounds
AUTHOR(S): Bock, Bodo; Kuhr, Manfred; Musso, Hans
CORPORATE SOURCE: Inst. Org. Chem., Univ. Karlsruhe, Karlsruhe, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1976), 109(3), 1184-94
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German

AB Magnetic anisotropies in mesityl and 9-anthryl derivs of benzene, mesitylene, anthracene, pyrimidine, pyrazole, and isoxazole were measured via 1H-NMR chem. shift data. The chem. shift differences of the 1-H and 4-H signals of 9-anthryl substituents are a measure of the magnetic anisotropy of arom. systems.

IT 55146-22-4
RL: PRP (Properties)
(NMR of)

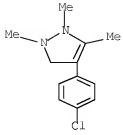
RN 59146-22-4 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(2,4,6-trimethylphenyl)- (CA INDEX NAME)



L11 ANSWER 32 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:175242 CAPLUS Full-text
DOCUMENT NUMBER: 82:175242
ORIGINAL REFERENCE NO.: 82:27995a,27998a
TITLE: Compositions of 1,2-dialkyl-3(and/or4)-aryl-3-pyrazolines and salts and method of lowering blood sugar levels with them
INVENTOR(S): Jacquier, Robert
PATENT ASSIGNEE(S): Schering A.-G., Fr.
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3818095	A	19740618	US 1972-243427	19720412

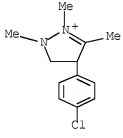
PRIORITY APPLN. INFO.: US 1972-243427 19720412
GI For diagram(s), see printed CA Issue.
AB 2-Pyrazolinium perchlorates (I) were prepd. and used in pharmaceutical compns. as hypoglycemics. Thus propiophenone [93-55-0], MeNHNHMe.2HCl [306-37-6], and HCHO [50-00-0] in EtOH with HCl were heated at reflux for 5 hr and worked up to give 1,2,4-trimethyl-3-phenyl-3-pyrazoline (II) [18508-29-7]. II (and other pyrazolines) were treated with HClO4 to give the perchlorate salts with a shift of the double bond to position 2. A tablet formulation contained, e.g., 50 mg/tablet 1,2,4-trimethyl-3-phenyl-2-pyrazolinium perchlorate [18075-75-7].
IT 51771-94-9P 51772-13-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51771-94-9 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl- (CA INDEX NAME)



RN 51772-13-5 CAPLUS
CN 1H-Pyrazolium, 4-(4-chlorophenyl)-4,5-dihydro-1,2,3-trimethyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 51772-12-4
CMF C12 H16 Cl N2



CM 2

CRN 14797-73-0
CMF Cl O4

L11 ANSWER 33 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:496468 CAPLUS Full-text
DOCUMENT NUMBER: 81:96468
ORIGINAL REFERENCE NO.: 81:15239a,15242a
TITLE: Compositions of 1,2-alkyl arylpyrazolium quaternary salts and lowering blood sugar levels with same

INVENTOR(S): Sherlock, Margaret
PATENT ASSIGNEE(S): Schering Corp.
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3818096	A	19740618	US 1972-243429	19720412

PRIORITY APPLN. INFO.: US 1972-243429 19720412

AB Compns. for lowering blood sugar levels in warm blooded animals suffering from hyperglycemia consist of a pharmaceutical carrier and I. Thus, to Ph3CCl in MeCN was added 1,2-dimethyl-3-phenyl-3-pyrazoline in MeCN to give after workupl,2-dimethyl-3-phenylpyrazolium chloride (II), m.p. 190-2.degree. (decompn.). Tablets are prepd. contg. II 100.00, confectioner's sugar (food grade) 123.00, polyvinylpyrrolidone (PVP) 10.00, corn starch (food grade, dried) 13.00, SiO2 2.00, and Mg sterate (U.S.P.) 2.00 mg/tablet. A damp mass consisting of II, the sugar, and PVP is prepd., dried, and reduced to granules. The starch, SiO2, and Mg stearate are added and mixed in. The compn. is then compressed into tablets.

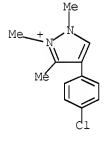
IT 54156-57-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(antihyperglycemic, prepn. of)

RN 54156-57-9 CAPLUS

CN 1H-Pyrazolium, 4-(4-chlorophenyl)-1,2,3-trimethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

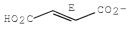
CRN 54156-56-8
CMF C12 H14 Cl N2



CM 2

CRN 18610-40-7
CMF C4 H3 O4

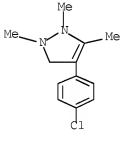
Double bond geometry as shown.



L11 ANSWER 34 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:120928 CAPLUS Full-text
DOCUMENT NUMBER: 80:120928
ORIGINAL REFERENCE NO.: 80:19467a,19470a
TITLE: Antiglycemic 3-pyrazolines
PATENT ASSIGNEE(S): Laboratoire Cetrane
SOURCE: Fr. Demande, 39 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2179559	A1	19731123	FR 1972-12761	19720412
FR 2179559	B1	19750425		
PRIORITY APPLN. INFO.:			FR 1972-12761	19720412

GI For diagram(s), see printed CA Issue.
AB Pyrazoles I, II, and III (R = Me, Ph, substituted phenyl; R1 = H, Me, Et, Ph, p-ClC6H4; R2 = H, Me, Ph; X = ClO4, iodide, fumarate) (56 compds.), were prepd. Condensation of RCOCHR1CH2R2 or RCOCHR1COR2 with MeNHNHMe.2HCl and paraformaldehyde gave I or II, resp. LiAlH4 redn. of II gave pyrazolinium III.
IT 51771-94-9P 51772-13-5P 51772-18-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51771-94-9 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl- (CA INDEX NAME)

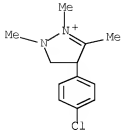


RN 51772-13-5 CAPLUS
CN 1H-Pyrazolium, 4-(4-chlorophenyl)-4,5-dihydro-1,2,3-trimethyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 51772-12-4

CMF C12 H16 Cl N2



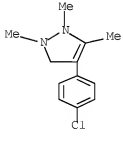
CM 2

CRN 14797-73-0
CMF Cl O4

RN 51772-18-0 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-2,3-dihydro-1,2,5-trimethyl-,
(2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 51771-94-9
CMF C12 H15 Cl N2

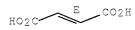


CM 2

CRN 110-17-8

CMF C4 H4 O4

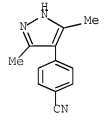
Double bond geometry as shown.



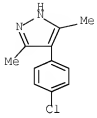
L11 ANSWER 35 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1974:108434 CAPLUS Full-text
DOCUMENT NUMBER: 80:108434
ORIGINAL REFERENCE NO.: 80:17443a,17446a
TITLE: Reactivity of 4-diazo-3,5-dimethylpyrazole. IV. Catalytic action of hydroquinone in the Gomberg-Bachmann reaction
AUTHOR(S): Fukata, Gouki; Kawazoe, Yuichi; Taguchi, Tanezo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, Japan
SOURCE: Yakugaku Zasshi (1974), 94(1), 36-43
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Refluxing 4-diazo-3,5-dimethylpyrazole (I) in benzene for a long time afforded 4-phenyl-3,5-dimethylpyrazole, 1H,4H-3-methylpyrazolo[4,3-c]-pyrazole, 3,5-dimethylpyrazole, and biphenyl in 36, 15, 12, and 7% yields, resp. Replacement of benzene with nitrobenzene in this reaction gave o-, m-, and p-isomers of 4-(nitrophenyl)-3,5-dimethylpyrazole in a ratio of 10:2.8:3.0. In these reactions, addn. of hydroquinone (catalytic quantity, 5% by wt. of I) was very effective in increasing the yield of 4-aryl-3,5-dimethylpyrazole and reduction of reaction time. The intermediate in these reactions was a diazonium salt which was formed by the addn. of one mole of hydroquinone to two moles of I.

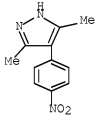
IT 51463-73-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in benzonitrile)
RN 51463-73-1 CAPLUS
CN Benzonitrile, 4-(3,5-dimethyl-1H-pyrazol-4-yl)- (CA INDEX NAME)



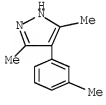
IT 51463-76-4P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in chlorobenzene)
RN 51463-76-4 CAPLUS
CN 1H-Pyrazole, 4-(4-chlorophenyl)-3,5-dimethyl- (CA INDEX NAME)



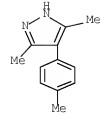
IT 42418-61-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in nitrobenzene)
RN 42418-61-1 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(4-nitrophenyl)- (CA INDEX NAME)



IT 51463-81-1P 51463-82-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by refluxing diazodimethylpyrazole in toluene)
RN 51463-81-1 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(3-methylphenyl)- (CA INDEX NAME)



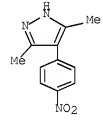
RN 51463-82-2 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(4-methylphenyl)- (CA INDEX NAME)



102b

Cited ref

L11 ANSWER 36 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1973:452480 CAPLUS Full-text
DOCUMENT NUMBER: 79:52480
ORIGINAL REFERENCE NO.: 79:8467a,8470a
TITLE: Reactivity of 4-diazo-3,5-dimethylpyrazole
AUTHOR(S): Fukata, Gouki; Kawazoe, Yuichi; Taguchi, Tanezo
CORPORATE SOURCE: Fac. Pharm. Sci., Kyushu Univ., Fukuoka, Japan
SOURCE: Tetrahedron Letters (1973), (15), 1199-200
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title compd. (I) was heated in Me3COH-AcOH, Me3COH, and EtOH to give 70% II, 45% III, and 85% MeCHO resp. Heating I in C6H6 gave 15% II, 12% 3,5-dimethylpyrazole, 7% biphenyl, and 36% IV. Hydroquinone and benzoquinone catalyzed the reaction giving IV (68%). III was also obtained by coupling I with II in Me3COH. Heating I in PhNO2 gave 4-nitrophenyl-3,5-dimethylpyrazole with a ratio of o:m:p-isomers = 10:3:3.
IT 42418-61-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 42418-61-1 CAPLUS
CN 1H-Pyrazole, 3,5-dimethyl-4-(4-nitrophenyl)- (CA INDEX NAME)



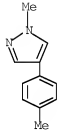
L11 ANSWER 37 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1972:539882 CAPLUS Full-text
DOCUMENT NUMBER: 77:139882
ORIGINAL REFERENCE NO.: 77:23001a,23004a
TITLE: Pyrazoles. IX. Nitration of 1-methyl-4-phenylpyrazole
AUTHOR(S): Cohen-Fernandes, Pauline; Habraken, Clarisse L.
CORPORATE SOURCE: Gorlaeus Lab., Univ. Leiden, Leiden, Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1972), 91(9-10), 1185-92
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English

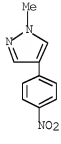
AB The phenyl and the pyrazole ring were both substituted on nitration with acetyl nitrate and a predominant ortho substitution in the phenyl ring was obsd. The pyrazole ring was susceptible to nitration at positions other than the, hitherto favored, 4-position.

IT 37921-11-2P 37921-15-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 37921-11-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-methylphenyl)- (CA INDEX NAME)



RN 37921-15-6 CAPLUS
CN 1H-Pyrazole, 1-methyl-4-(4-nitrophenyl)- (CA INDEX NAME)



L11 ANSWER 38 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:46687 CAPLUS Full-text
DOCUMENT NUMBER: 58:46687
ORIGINAL REFERENCE NO.: 58:7921a-c
TITLE: Derivatives of 3-substituted pyrazolones and 3-substituted pyrazolines
AUTHOR(S): Kurihara, Tozaburo; Takeda, Hideo; Iino, Naoko
CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai
SOURCE: Tohoku Yakka Daigaku Kiyo (1961), 8, 103-9
CODEN: TYDKAG; ISSN: 0372-347X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB 1-Phenyl-3-chloro-4-pyrazoolone (1.9 g.) was warmed with 0.9 g. Me2NH in MeOH in an autoclave 2 hrs. to give 1-phenyl-3-dimethylamino-5-pyrazolone, m. 132.degree. (EtOH). Similarly prepd. were the following I (R, R1, R2, and m.p. given): H, H, NEt2, 131.degree.; H, H, (iso-Bu)2 N, 108.degree.; H, Br, (iso-Bu)2 N, 138-40.degree.; H, Cl, (iso-Bu)2N, 126.degree.; H, H, piperidyl, 139.degree.; H,H, morpholyl, 134.degree.; Bu, H, morpholyl, 225.degree.; H, Br, morpholyl, 165.degree.; H, Cl, morpholyl, 143.degree.; H. Me, morpholyl, 168-170.degree.; H, OMe, morpholyl, 127-30.degree.; H, H, Et2NCH2NH, 202.degree.; H, H, Et2NCH2CONH, 158.degree.; H, H, morpholylacetamido.

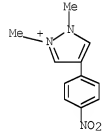
IT 94628-08-7
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 94628-08-7 CAPLUS

CN 1H-Pyrazolium, 1,2-dimethyl-4-(4-nitrophenyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 94628-07-6
CMF C11 H12 N3 O2



CM 2

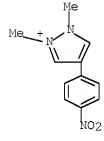
CRN 14797-73-0
CMF Cl O4

L11 ANSWER 39 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:46686 CAPLUS Full-text
DOCUMENT NUMBER: 58:46686
ORIGINAL REFERENCE NO.: 58:7920h,7921a
TITLE: The 1,2-dithiolium cation. A new pseudoaromatic system. III. Conversion of dithiolium salts to quaternary pyrazolium salts and dithiolethiones
AUTHOR(S): Klingsberg, Erwin

CORPORATE SOURCE: Am. Cyanamid Co., Bound Brook, NJ
SOURCE: Journal of Organic Chemistry (1963), 28, 529-30
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:46686
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 16791e. 4-Phenyl-(I) and 4-p-nitrophenyl-1,2-dithiolium salts react with N,N'-disubstituted hydrazines to give N,N-disubstituted pyrazolium salts, e.g., II, and with sulfur to give 1,2-dithiole-3-thiones, e.g. III.
IT 94628-08-7P, 1,2-Dimethyl-4-(p-nitrophenyl)pyrazolium perchlorate
RL: PREP (Preparation)
(prepn. of)
RN 94628-08-7 CAPLUS
CN 1H-Pyrazolium, 1,2-dimethyl-4-(4-nitrophenyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 94628-07-6
CMF C11 H12 N3 O2



CM 2

CRN 14797-73-0
CMF Cl O4

L11 ANSWER 40 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:55872 CAPLUS Full-text
DOCUMENT NUMBER: 52:55872
ORIGINAL REFERENCE NO.: 52:10061i,10062a-c
TITLE: Synthesis of 2-substituted-acenaphtheno(4',5'-4,5)imidazole derivatives
AUTHOR(S): Saikachi, Haruo; Tsuge, Otohiko; Yoshimura, Kazuki

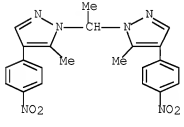
CORPORATE SOURCE: Kyushu Univ., Fukuoka
SOURCE: Kogyo Kagaku Zasshi (1956), 59, 933-6
CODEN: KGKZA7; ISSN: 0368-5462
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 52, 3779e. 4-Nitro-5-acylaminoacenaphthenes (I) (formyl, m. 226-7.degree.; Ac, 241.5-2.0.degree.; Bz, 228-9.degree.) were obtained from 5-amino-acenaphthene through the 5-acylaminoacenaphthene. Formyl and Ac derivs. of I were hydrolyzed by heating with EtOH-HCl 20 hrs. to give 4-nitro-5-aminoacenaphthene (II), m. 212-13.degree.. II was reduced with SnCl in HCl satd. EtOH to give 4,5-diaminoacenaphthene (III), m. 137.degree.. III (1 g.) with 3 cc. boiling 80% HCO2H gave 0.6 g. acenaphtheno(4',5'-4,5)imidazole, m. 221-2.degree.. III (1 g.) with 2 cc. Ac2O in C6H6 on an H2O bath gave 0.6 g. 1-(N-acetyl)-2-methyl-acenaphtheno(4',5'-4,5)imidazole (IV), m. 263.degree.. Ac deriv. of I was reduced in Ac2O by Zn and converted to IV. The reduction of formyl deriv. of I in Ac2O with Zn by boiling gave 1-(N-carboxy) - 2 - methylacenaphtheno(4',5' - 4,5)imidazole, m. 279.degree., sol. in aq. NaOH. 4,5-Dibenzoyldiaminoacenaphthene, m. 282-3.degree., was obtained by boiling III with BzCl. III.HCl (1 g.) heated with 0.3 g. urea at 150-5.degree. 45 min. and extd. with aq. NaOH and then EtOAc gave acenaphtheno-(4',5'-4,5)-2-imidazolinone, m. above 340.degree.. Similarly, III.HCl with thiourea at 230.degree. or 450.degree. gave acenaphtheno-(4',5'-4,5)-2-thioimidazolinone, m. above 340.degree..

IT 102599-03-1P, Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)-
RL: PREP (Preparation)
(prepn. of)

RN 102599-03-1 CAPLUS

CN Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)- (6CI) (CA INDEX NAME)



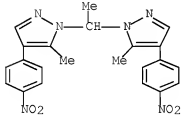
L11 ANSWER 41 OF 41 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1958:55871 CAPLUS Full-text
DOCUMENT NUMBER: 52:55871
ORIGINAL REFERENCE NO.: 52:10061e-i
TITLE: Products from the reaction of diazoethane with diazoketones
AUTHOR(S): Yates, P.; Farnum, D. G.; Wiley, D. W.
CORPORATE SOURCE: Harvard Univ.
SOURCE: Chemistry & Industry (London, United Kingdom) (1958) 69-70
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 43, 4652g, 6992e. The structures ArCOCR:NN:CHR' (R = R' = Me) (I) and (R = H, R' = Me) (II) (Ar = p-O2NC6H4 throughout) previously proposed (C.A. 43, 6992e) for the products of the reaction between ARCOCRN2 and MeCHN2 were confirmed. I, m. 99-100.degree., .lambda. 265 m.mu. (.epsilon. 13,700), .lambda. 5.93, 6.06, 6.23 .mu., boiled 15 min. with 70% EtOH gave (ArCOCMe:NNH)2CHMe (III), m. 159-60.degree., .lambda. 268 and 315 m.mu. (.epsilon. 35,300 and 18,900), .lambda. 3.04, 6.03 (shoulder), 6.06, 6.24, 6.39 .mu., corresponding to the earlier compd., C11H9O2N3 (C.A. 43, 6992e). III with Ac2O and NaOAc gave ArCOCMe:NNHAc, m. 165.5-6.5.degree., .lambda. 245 and 278 m.mu. (.epsilon. 12,100 and 19,300), .lambda. 3.04, 5.81, 5.92, 5.99, 6.26 .mu., identical with the acetylated product of ArCOCMe:NNH2 (IV), m. 173-3.2.degree., .lambda. 274 m.mu. (.epsilon. 14,200), .lambda. 2.92, 3.03, 3.31, 6.04, 6.16, 6.25, 6.36 .mu., obtained by NH4HS reduction of ArCOCMeN2. III with BzH gave ArCOCMe:NN:CHPh, m. 114.5-15.5.degree., .lambda. 5.98, 6.18, 6.23, 6.40 .mu., also obtained from IV. I with IV 6 days in CHCl3 or refluxing in abs. EtOH gave III (63% yield by the 2nd method). I heated alone in abs. EtOH gave ArCOCMe:NNHCHMeOEt, m. 126-7.degree., .lambda. 268 and 305 m.mu. (.epsilon. 17,750 and 11,000), .lambda. 3.03, 6.08, 6.24, 6.42 .mu., which was converted to III by treatment with aq. EtOH. ArCOCHN2 with MeCHN2 gave the 2 stereoisomers of II, A, m. 69-70.degree., .lambda. 5.93, 6.09, 6.22 .mu., B, m. 121-2.degree. (decompn.), .lambda. 5.99, 6.09, 6.24, 6.29 .mu.; A was converted to B by heating at its m.p. Further reaction of II with MeCHN2 gave ArCOCMe:CHNHN:CHMe (V), m. 136-6.5..degree., .lambda. 298 m.mu. (.epsilon. 22,800), .lambda. 3.02, 6.08, 6.16, 6.31 .mu., corresponding to the earlier compd. (C.A. 43, 6992e), C14H17O3N3. Hydrolysis of V in cold 2N HCl gave 3-(p-nitrophenyl)-4-methylpyrazole (VI), m. 181.5-2.degree., .lambda. 2.92, 3.13, 6.23 .mu., identified by nitration of the Ph analog, and [ArC:CMe.CH:N.N]2CHMe, m. 201.5-2.5.degree., .lambda. 231 and 318 m.mu. (.epsilon. 22,500 and 21,800), .lambda. 6.24 and 6.44 .mu.. Ultraviolet spectra were taken in CH2Cl2, infrared spectra in CHCl3.

IT 102599-03-1P, Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)-
RL: PREP (Preparation)
(prepn. of)

RN 102599-03-1 CAPLUS

CN Pyrazole, 1,1'-ethylidenebis[5-methyl-4-(p-nitrophenyl)- (6CI) (CA INDEX NAME)



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Executing the logoff script...

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	71.18	327.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-9.84	-9.84

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STN INTERNATIONAL SESSION SUSPENDED AT 10:38:43 ON 24 APR 2009